



Contents lists available at ScienceDirect

Linear Algebra and its Applications

journal homepage: www.elsevier.com/locate/laa



Detecting hyperbolic and definite matrix polynomials

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ARTICLE INFO

Article history:

Received 22 April 2008

Accepted 18 September 2009

Available online 17 November 2009

Submitted by V. Mehrmann

AMS classification:

15A18

15A24

65F15

65F30

Keywords:

Matrix polynomial

Quadratic eigenvalue problem

Definite matrix polynomial

Hyperbolic

Overdamped

Minmax characterization

Safeguarded iteration

ABSTRACT

Hyperbolic or more generally definite matrix polynomials are important classes of Hermitian matrix polynomials. They allow for a definite linearization and can therefore be solved by a standard algorithm for Hermitian matrices. They have only real eigenvalues which can be characterized as minmax and maxmin values of Rayleigh functionals, but there is no easy way to test if a given polynomial is hyperbolic or definite or not. Taking advantage of the safeguarded iteration which converges globally and monotonically to extreme eigenvalues we obtain an efficient algorithm that identifies hyperbolic or definite polynomials and enables the transformation to an equivalent definite linear pencil. Numerical examples demonstrate the efficiency of the approach.

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1. Introduction

The polynomial eigenvalue problem $P(\lambda)x = 0$ with

$$P(\lambda) = \sum_{j=0}^{\ell} \lambda^j A_j, \quad A_j \in \mathbb{C}^{n \times n}, \quad A_{\ell} \neq 0 \quad (1.1)$$

arises in a variety of applications and is an active subject of research. Most important in practice is the quadratic case (cf. [31] for a recent survey)

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$$Q(\lambda) := \lambda^2 A + \lambda B + C, \quad A, B, C \in \mathbb{C}^{n \times n}, A \neq 0, \quad (1.2)$$

but higher degrees also occur in applications [1,13–17,26,28,30,32].

A standard approach to treating the polynomial eigenvalue problem (1.1) both theoretically and numerically is linearization, i.e. to transform (1.1) into an equivalent linear eigenvalue problem $L(\lambda)X = \lambda GX - HX = 0$ where $G, H \in \mathbb{C}^{n\ell \times n\ell}$ and $X \in \mathbb{C}^{n\ell}$ which then can be solved by a standard eigenvalue solver such as the QZ algorithm or the Cholesky-QR algorithm if $L(\lambda)$ is a definite Hermitian pencil, i.e. G and H are Hermitian and some linear combination is positive definite. Most widely used in practice are companion forms one of which is

$$L(\lambda) = \lambda \begin{pmatrix} A_\ell & 0 & \dots & 0 \\ 0 & I_n & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \dots & 0 & I_n \end{pmatrix} + \begin{pmatrix} A_{\ell-1} & A_{\ell-2} & \dots & A_0 \\ -I_n & 0 & \dots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \dots & -I_n & 0 \end{pmatrix}. \quad (1.3)$$

They are easily constructed, but their disadvantage is that structural properties such as symmetry are not preserved.

Mackey et al. [23] introduced an approach to constructing linearizations of polynomial eigenvalue problems which generalizes the companion forms, and which gave rise to linearizations preserving symmetry [10] and respecting palindromic and odd-even structures [22].

In a recent paper Higham et al. [11] studied Hermitian matrix polynomials (i.e. $A_j = A_j^H$ for $j = 0, \dots, \ell$) which allow for a definite linearization. They proved that (in a certain class of linearizations) these are characterized by the properties that there exists $\mu \in \mathbb{R} \cup \{\infty\}$ such that $P(\mu)$ is positive definite and for every $x \in \mathbb{C}^n$, $x \neq 0$ the scalar polynomial $q(\lambda; x) := x^H P(\lambda)x$ has ℓ distinct roots in $\mathbb{R} \cup \{\infty\}$. These Hermitian matrix polynomial are called definite.

Moreover, it was proved in [11] that a matrix polynomial is definite if and only if there exist $\gamma_j \in \mathbb{R} \cup \{\infty\}$ with $\gamma_0 > \gamma_1 > \dots > \gamma_{\ell-1}$ ($\gamma_0 = \infty$ being possible) such that $P(\gamma_j)$, $j = 0, \dots, \ell - 1$ are alternately positive and negative definite. If parameters γ_j with this property are known then a set of definite linearizations of $P(\lambda)$ can be given explicitly. Once this definite linearization is known it can be reduced to a standard Hermitian eigenproblem using the Cholesky factorization and solved by a standard solver for Hermitian eigenvalue problems. However, no easy way was known to test if a given matrix polynomial is definite and how to construct the γ_j s.

Definite matrix polynomials generalize hyperbolic matrix polynomials which are defined by the requirements that A_ℓ is positive definite (and so is $P(\mu)$ if μ is sufficiently large) and that the scalar polynomial $q(\lambda; x)$ has ℓ distinct real roots for every $x \neq 0$ (cf. [6]).

For quadratic hyperbolic pencils Higham et al. [12] proposed a method for testing hyperbolicity and for constructing a definite linearization. Another method for detecting if a Hermitian quadratic matrix polynomial is hyperbolic which is based on cyclic reduction was introduced by Guo and Lancaster [9] and was accelerated by Guo et al. [7], and a further method based on an improved arc algorithm for a Hermitian linearization of the quadratic pencil is studied in [7].

In this paper we take advantage of the fact that all eigenvalues of a definite matrix polynomial can be characterized as minmax values of appropriate Rayleigh functionals and that the extreme eigenvalues in each of the intervals $(-\infty, \gamma_{\ell-1})$, (γ_j, γ_{j-1}) , $j = \ell - 1, \dots, 1$, and (γ_0, ∞) are the limits of monotonically and quadratically convergent sequences, and we design a method to decide whether a given Hermitian matrix polynomial is definite. In the affirmative case we concurrently determine parameters γ_j such that the matrices $P(\gamma_j)$ are alternately positive and negative definite, which allows for the construction of a definite linearization.

Our paper is organized as follows. In Chapter 2 we provide our basic tools: a minmax characterization of eigenvalues of certain nonlinear Hermitian eigenvalue problems, and the safeguarded iteration which for this type of problems converges globally and monotonically to extreme eigenvalues. The following chapters are devoted to the algorithm for detecting hyperbolicity and definiteness, respectively, and for computing appropriate γ_j s for hyperbolic quadratic pencils in Chapter 3, general definite quadratic pencils in Chapter 4, hyperbolic matrix polynomials of higher degree in Chapter 5, and

its generalization to definite pencils of higher degree in Chapter 6. Numerical examples demonstrate the efficiency of our approach.

2. Preliminaries

Our main tools in this paper are variational characterizations of eigenvalues of nonlinear eigenvalue problems generalizing the well known minmax characterization of Poincaré [27] or Courant [2] and Fischer [5] for linear eigenvalue problems.

We consider the nonlinear eigenvalue problem

$$T(\lambda)x = 0, \quad (2.1)$$

where $T(\lambda) \in \mathbb{C}^{n \times n}$, $\lambda \in J$, is a family of Hermitian matrices depending continuously on the parameter $\lambda \in J$, and J is a real open interval which may be unbounded.

To generalize the variational characterization of eigenvalues we need a generalization of the Rayleigh quotient. To this end we assume that

(A₁) for every fixed $x \in \mathbb{C}^n$, $x \neq 0$ the real equation

$$f(\lambda; x) := x^H T(\lambda)x = 0 \quad (2.2)$$

has at most one solution $p(x) \in J$.

Then $f(\lambda; x) = 0$ defines a functional p on some subset $\mathcal{D}(p) \subset \mathbb{C}^n$ which is called the Rayleigh functional of (2.1), and which is exactly the Rayleigh quotient in case of a monic linear matrix function $T(\lambda) = \lambda I - A$.

Generalizing the definiteness requirement for linear pencils $T(\lambda) = \lambda B - A$ we further assume that

(A₂) for every $x \in \mathcal{D}(p)$ and every $\lambda \in J$ with $\lambda \neq p(x)$ it holds that

$$(\lambda - p(x))f(\lambda; x) > 0. \quad (2.3)$$

Under these conditions the following characterizations of extreme eigenvalues hold. A more general version of this result is contained in [34,35]. In accordance with these papers we call $\lambda_j \in J$ a j th eigenvalue of $T(\cdot)$ if $\mu = 0$ is a j th largest eigenvalue of the linear eigenvalue problem $T(\lambda_j)x = \mu x$.

Theorem 2.1. *Let J be an open interval in \mathbb{R} , and let $T(\lambda) \in \mathbb{C}^{n \times n}$, $\lambda \in J$, be a family of Hermitian matrices depending continuously on the parameter $\lambda \in J$ such that the conditions (A₁) and (A₂) are satisfied.*

(i) *Assume that*

$$\lambda_1 := \inf_{x \in \mathcal{D}(p), x \neq 0} p(x) \in J, \quad (2.4)$$

and that there exists a k -dimensional subspace $W \subset \mathbb{C}^n$ such that $W \cap \mathcal{D}(p) \neq \emptyset$ and

$$\sup_{x \in W \cap \mathcal{D}(p)} p(x) \in J. \quad (2.5)$$

Then for $j = 1, \dots, k$ there exists a j th eigenvalue $\lambda_j \in J$, it holds that

$$\lambda_j = \min_{\dim V=j, V \cap \mathcal{D}(p) \neq \emptyset} \max_{x \in V \cap \mathcal{D}(p)} p(x), \quad j = 1, \dots, k, \quad (2.6)$$

and there exist no further eigenvalues of $T(\cdot)$ in J less than λ_k . If the minimum in (2.6) is attained for some subspace V then $V \subset \mathcal{D}(p) \cup \{0\}$.

(ii) Assume that

$$\lambda_n := \sup_{x \in \mathcal{D}(p), x \neq 0} p(x) \in J, \quad (2.7)$$

and that there exists a k -dimensional subspace $W \subset \mathbb{C}^n$ such that $W \cap \mathcal{D}(p) \neq \emptyset$ and

$$\inf_{x \in W \cap \mathcal{D}(p)} p(x) \in J. \quad (2.8)$$

Then for $j = 1, \dots, k$ there exists a $(n - j + 1)$ th eigenvalue $\lambda_{n-j+1} \in J$, it holds that

$$\lambda_{n-j+1} = \max_{\dim V=j, V \cap \mathcal{D}(p) \neq \emptyset} \min_{x \in V \cap \mathcal{D}(p)} p(x), \quad j = 1, \dots, k, \quad (2.9)$$

and there exist no further eigenvalues of $T(\cdot)$ in J greater than λ_{n-k+1} . If the maximum in (2.9) is attained for some subspace V then $V \subset \mathcal{D}(p) \cup \{0\}$.

In particular, if $\inf_{x \in \mathcal{D}(p)} p(x) \in J$ and $\sup_{x \in \mathcal{D}(p)} p(x) \in J$, then $\mathcal{D}(p) \cup \{0\} = \mathbb{C}^n$, and J contains exactly n eigenvalues of $T(\cdot)$ which can be characterized as minmax and maxmin values of the Rayleigh functional p . For this so called overdamped case the minmax and maxmin characterizations were already proved by Duffin [4] for quadratic eigenvalue problems, and by Rogers [29] for the general problem (2.1) (assuming the sufficient condition for (A_2) that $T(\lambda)$ is differentiable in J , and $x^H T'(p(x))x > 0$ for $x \neq 0$).

The proof of (2.6) reveals that the subspace for which the minimum in (2.6) is attained is the invariant subspace of $T(\lambda_j)$ which is spanned by the eigenvectors of the matrix $T(\lambda_j)$ corresponding to its j th largest eigenvalues, and that the maximum is attained for every eigenvector of $T(\lambda_j)$ corresponding to its eigenvalue $\mu = 0$. This suggests the following method called safeguarded iteration for computing the j th eigenvalue of $T(\cdot)$.

Algorithm 1. Safeguarded iteration:

This algorithm computes the j th smallest eigenvalue σ and corresponding eigenvector x of a nonlinear eigenvalue problem $T(\lambda)x = 0$ with Rayleigh functional p

Require: initial vector $x_0 \in \mathcal{D}(p)$

1: compute $\sigma_0 = p(x_0)$

2: **for** $k = 1, 2, \dots$ until convergence **do**

3: determine an eigenvector x_k corresponding to the j th largest eigenvalue of $T(\sigma_{k-1})$

4: determine Rayleigh functional $\sigma_k := p(x_k)$, i.e. solve $x_k^H T(\sigma_k)x_k = 0$ for σ_k

5: **end for**

6: $\sigma := \sigma_k, x := x_k$

The following theorem contains the convergence properties of the safeguarded iteration. It was already proved in [36] but because this technical report is not easily available we repeat its proof here.

Theorem 2.2. Let $J \subset \mathbb{R}$ be an open interval, let $T(\lambda) \in \mathbb{C}^{n \times n}, \lambda \in J$, be a family of Hermitian matrices depending continuously on the parameter $\lambda \in J$ such that the conditions (A_1) and (A_2) are satisfied.

- (i) If $\lambda_1 := \inf_{x \in \mathcal{D}(p)} p(x) \in J$ and $x_0 \in \mathcal{D}(p)$ then the safeguarded iteration for $j = 1$ converges globally and is monotonically decreasing to λ_1 .
- (ii) If $T(\lambda)$ is holomorphic on a neighborhood $U \subset \mathbb{C}$ of a j th eigenvalue of $T(\cdot)$ and λ_j is a simple eigenvalue, then the safeguarded iteration converges locally and quadratically to λ_j .
- (iii) Under the conditions of (ii) the local convergence of the safeguarded iteration is even cubic if $T'(\lambda)$ is positive definite for $\lambda \in U \cap J$, and x_k in step 3 of Algorithm 1 is chosen to be an eigenvector corresponding to the j th largest eigenvalue of the generalized eigenproblem $T(\sigma_{k-1})x = \mu T'(\sigma_{k-1})x$ with $\sigma_{k-1} = p(x_{k-1})$.

Proof. We assume that all iterates x_k are normalized such that $\|x_k\| = 1$, where $\|\cdot\|$ denotes the 2-norm.

(i) Let $\sigma_{k-1} \geq \lambda_1$. Then it holds that

$$\mu_n(\sigma_{k-1}) := \max_{x \neq 0} \frac{x^H T(\sigma_{k-1})x}{x^H x} = x_k^H T(\sigma_{k-1})x_k \geq x_{k-1}^H T(\sigma_{k-1})x_{k-1} = 0, \quad (2.10)$$

where $\mu_n(\sigma)$ denotes the maximal eigenvalue of $T(\sigma)$. Suppose that $x_k \notin \mathcal{D}(p)$. Then it follows from (2.10) that $x_k^H T(\lambda)x_k > 0$ for every $\lambda \in J$.

Let $\tilde{x} \in \mathcal{D}(p)$ be an eigenvector of T corresponding to λ_1 . Then we get from (A_2) $\tilde{x}^H T(\lambda)\tilde{x} < 0$ for every $\lambda \in J, \lambda < \lambda_1$. Hence for fixed $\lambda \in J, \lambda < \lambda_1$

$$q(t) := (\tilde{x} + t(x_k - \tilde{x}))^H T(\lambda)(\tilde{x} + t(x_k - \tilde{x})) = 0$$

has a solution $\tilde{t} \in (0, 1)$, i.e. $w := \tilde{x} + \tilde{t}(x_k - \tilde{x}) \in \mathcal{D}(p)$ and $p(w) = \lambda < \lambda_1$ contradicting (2.4).

The monotonicity of $\{\sigma_k\}$ follows directly from the definition of σ_{k+1} , (2.10) and (A_2) . Let $\hat{\sigma} := \lim_{k \rightarrow \infty} \sigma_k$ and let $\{x_{k_i}\}$ be a convergent subsequence of $\{x_k\}$, $x_{k_i} \rightarrow \hat{x} \neq 0$. Then by the continuity of $T(\lambda)$

$$0 = x_{k_i}^H T(\sigma_{k_i})x_{k_i} \rightarrow \hat{x}^H T(\hat{\sigma})\hat{x},$$

i.e. $\hat{x} \in \mathcal{D}(p)$ and $p(\hat{x}) = \hat{\sigma}$, and we get from the continuous dependence of $\mu_n(\sigma)$ on σ

$$T(\hat{\sigma})\hat{x} = \lim_{i \rightarrow \infty} T(\sigma_{k_i-1})x_{k_i} = \lim_{i \rightarrow \infty} \mu_n(\sigma_{k_i-1})x_{k_i} = \mu_n(\hat{\sigma})\hat{x}.$$

Multiplying this equation by \hat{x}^H yields $\mu_n(\hat{\sigma}) = 0$, and hence $\hat{\sigma} = \lambda_1$.

(ii) If λ_j is a simple eigenvalue of $T(\cdot)$ then it is an easy consequence of the implicit function theorem that for $|\lambda - \lambda_j|$ small enough the function $\lambda \mapsto x(\lambda)$ is defined and continuously differentiable, where $x(\lambda)$ denotes the suitably normalized eigenvector of $T(\lambda)$ corresponding to the j th largest eigenvalue. Because $\mathcal{D}(p)$ is an open set, $h(\lambda) := p(x(\lambda))$ is defined in a neighborhood of λ_j , and since the eigenvectors of $T(\cdot)$ are the stationary points of p , we get

$$h'(\lambda_j) = p'(x(\lambda_j))x'(\lambda_j) = 0.$$

This proves the quadratic convergence of $\sigma_{j+1} = h(\sigma_j)$ to λ_j .

(iii) Let $T'(\lambda)$ be positive definite and denote by $\mu(\lambda)$ the j th largest eigenvalue of the generalized eigenproblem $T(\lambda)x = \mu T'(\lambda)x$ and by $x(\lambda)$ a corresponding eigenvector which is suitably normalized such that $x(\cdot)$ is continuous. If λ_j is a j th eigenvalue of $T(\cdot)$ then $\mu(\lambda_j) = 0$, and differentiating $T(\lambda)x(\lambda) = \mu(\lambda)T'(\lambda)x(\lambda)$ yields

$$T'(\lambda_j)x(\lambda_j) + T(\lambda_j)x'(\lambda_j) = \mu'(\lambda_j)T'(\lambda_j)x(\lambda_j).$$

Multiplying by $x(\lambda_j)^H$ from the left we get $\mu'(\lambda_j) = 1$, and therefore

$$T(\lambda_j)x'(\lambda_j) = 0. \quad (2.11)$$

If we define h analogously to part (ii) by $h(\lambda) = p(x(\lambda))$ then as before $h'(\lambda_j) = 0$, and from

$$h''(\lambda_j) = -2 \frac{x'(\lambda_j)^H T(p(x(\lambda_j)))x'(\lambda_j)}{x(\lambda_j)^H T'(p(x(\lambda_j)))x(\lambda_j)}$$

and (2.11) it follows that $h''(\lambda_j) = 0$, i.e. the safeguarded iteration converges cubically. \square

It is obvious that the safeguarded iteration aiming at an n th eigenvalue $\lambda_n = \sup_{x \in \mathcal{D}(p)} p(x)$ converges globally and monotonically increasing to $\lambda_n \in J$ if $x_0 \in \mathcal{D}(p)$.

If $T(\lambda) \in \mathbb{R}^{n \times n}$ is a real symmetric family of matrices, then the quadratic and cubic convergence in (ii) and (iii) is valid if $T(\cdot)$ is differentiable and twice differentiable, and the first and second derivative is Lipschitz continuous, respectively.

3. Hyperbolic quadratic eigenvalue problems

Consider the hyperbolic quadratic eigenvalue problem

$$Q(\lambda)x := (\lambda^2 A + \lambda B + C)x = 0, \quad (3.1)$$

where $A, B, C \in \mathbb{C}^{n \times n}$ are Hermitian, $A > 0$ (i.e. A is positive definite), and for every $x \in \mathbb{C}^n, x \neq 0$ the quadratic polynomial

$$\lambda^2 x^H A x + \lambda x^H B x + x^H C x = 0 \quad (3.2)$$

has two distinct real roots

$$p_{\pm}(x) = \frac{-x^H B x \pm \sqrt{(x^H B x)^2 - 4(x^H A x)(x^H C x)}}{2x^H A x}. \quad (3.3)$$

The ranges $J_{\pm} := p_{\pm}(\mathbb{C}^n \setminus \{0\})$ are disjoint real intervals with $\max J_- < \min J_+$ (this was proved by Duffin [4] for the overdamped case, and this is true for hyperbolic problems as well since the shifted pencil $Q(\lambda + \theta)$ is overdamped for sufficiently large θ), $Q(\lambda)$ is positive definite for $\lambda < \min J_-$ and $\lambda > \max J_+$, and it is negative definite for $\lambda \in (\max J_-, \min J_+)$.

Each of the intervals J_- and J_+ contains n eigenvalues

$$\lambda_n^- \leq \lambda_{n-1}^- \leq \dots \leq \lambda_1^- < \lambda_1^+ \leq \dots \leq \lambda_n^+ \quad (3.4)$$

(notice that in J_- the sign condition (A_2) is satisfied for $-Q(\lambda)$, and therefore the smallest eigenvalue is an n th eigenvalue) which can be characterized as (cf. [4])

$$\lambda_j^- = \max_{\dim V=j} \min_{x \in V, x \neq 0} p_-(x), \quad \lambda_j^+ = \min_{\dim V=j} \max_{x \in V, x \neq 0} p_+(x).$$

The safeguarded iteration for λ_1^+ and λ_1^- converges globally and monotonically and is decreasing and increasing, respectively, for every initial vector $x_0 \in \mathbb{C}^n \setminus \{0\}$.

Algorithm 2. Hyperbolicity test for quadratic matrix polynomials

This algorithm tests whether a Hermitian quadratic pencil $Q(\lambda)$ is hyperbolic, and, if it is, computes μ such that $Q(\mu)$ is negative definite

Require: initial vector $x_0 \neq 0, \epsilon > 0$

- 1: **if** $d(x_0) = (x_0^H B x_0)^2 - 4(x_0^H A x_0)(x_0^H C x_0) < 0$ **then**
- 2: STOP: $Q(\lambda)$ is not hyperbolic
- 3: **end if**
- 4: determine $\sigma_0 = p_+(x_0)$
- 5: **for** $k = 1, 2, \dots$ **until** convergence **do**
- 6: determine eigenvector x_k of $Q(\sigma_{k-1})$ corresponding to its largest eigenvalue
- 7: **if** $d(x_k) = (x_k^H B x_k)^2 - 4(x_k^H A x_k)(x_k^H C x_k) < 0$ **then**
- 8: STOP: $Q(\lambda)$ is not hyperbolic
- 9: **end if**
- 10: determine $\sigma_k = p_+(x_k)$
- 11: **if** $|(\sigma_k - \sigma_{k-1})/\sigma_k| \leq \epsilon$ **then**
- 12: set $\sigma = \sigma_k, \omega_0 = p_-(x_k)$ and GOTO 2
- 13: **else if** $\sigma_k > \sigma_{k-1}$ **then**
- 14: STOP: $Q(\lambda)$ is not hyperbolic
- 15: **else if** $Q(2\sigma_k - \sigma_{k-1})$ is negative definite **then**

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16:    $\mu = 2\sigma_k - \sigma_{k-1}$ 
17:   STOP:  $Q(\lambda)$  is hyperbolic
18: end if
19: end for
20: for  $k = 1, 2, \dots$  until convergence do
21:   if  $Q((\omega_{k-1} + \sigma)/2)$  is negative definite then
22:      $\mu = (\omega_{k-1} + \sigma)/2$ 
23:     STOP:  $Q(\lambda)$  is hyperbolic
24:   else if  $|(\sigma - \omega_{k-1})/\omega_{k-1}| \leq \epsilon$  then
25:     STOP: Hyperbolicity not detectable,  $Q(\lambda)$  maybe weakly hyperbolic
26:   end if
27:   determine eigenvector  $x_k$  of  $Q(\omega_{k-1})$  corresponding to its largest eigenvalue
28:   if  $d(x_k) = (x_k^H B x_k)^2 - 4(x_k^H A x_k)(x_k^H C x_k) < 0$  then
29:     STOP:  $Q(\lambda)$  is not hyperbolic
30:   end if
31:   determine  $\omega_k = p_-(x_k)$ 
32:   if  $\omega_k < \omega_{k-1}$  then
33:     STOP:  $Q(\lambda)$  is not hyperbolic
34:   end if
35: end for

```

This suggests Algorithm 2 for testing whether $Q(\lambda)$ is hyperbolic. In the upper sweep (lines 1–19) we determine sequences x_k and $\sigma_k := p_+(x_k)$ by the safeguarded iteration for p_+ aiming at λ_1^+ which is terminated if a discriminant $d(x_k) = (x_k^T B x_k)^2 - 4(x_k^T A x_k)(x_k^T C x_k)$ is negative (indicating that $Q(\lambda)$ is not hyperbolic) or a parameter μ is found with $Q(\mu) < 0$ (indicating that $Q(\lambda)$ is hyperbolic).

If the relative distance of σ_k and σ_{k-1} becomes very small and hyperbolicity is not disclosed in line 15, we determine in the lower sweep (lines 20–35) sequences x_k and $\omega_k = p_-(x_k)$ by the safeguarded iteration for p_- aiming at λ_1^- . If there is a clear gap between J_- and J_+ , i.e. if $Q(\lambda)$ is hyperbolic, the matrix $Q(\mu)$, $\mu := 0.5(\min_j \sigma_j + \omega_k)$ will be negative definite after a few steps. However, it may happen that $\{\omega_k\}$ approaches $\min_j \sigma_j$ signalling that the gap is extremely small or even $\lambda_1^- = \lambda_1^+$.

Some further remarks about Algorithm 2 are in order.

- Since σ_k is evaluated by $\sigma_k = p_+(x_k)$ and the Rayleigh functional has similar approximation properties as the Rayleigh quotient in the linear case (i.e. an approximation x_k to an eigenvector with error $\mathcal{O}(\epsilon)$ yields an approximation $\sigma_k = p_+(x_k)$ to the corresponding eigenvalue the error of which satisfies $\mathcal{O}(\epsilon^2)$) the eigenvector approximations x_k do not have to be computed very accurately.
- Non-hyperbolicity is noticed in lines 1, 7, and 28, if the discriminant $d(x_k)$ is negative, and in lines 13 and 32 if the sequence σ_k and ω_k is not monotonically decreasing and increasing, respectively.
- Hyperbolicity is detected if $Q(\lambda)$ is negative definite for some λ . If λ_1^+ is a simple eigenvalue then the safeguarded iteration converges quadratically, and therefore (at least close to convergence) the increment $\rho_k := \sigma_{k-1} - \sigma_k$ will be greater than the error $\sigma_k - \lambda_1^+$. Moreover, ρ_k will converge to 0, and even if the gap $\lambda_1^+ - \lambda_1^-$ is small, a double step $\sigma_{k-1} + 2\rho_k = 2\sigma_k - \sigma_{k-1}$ is likely to hit the gap eventually. Therefore in line 15 the negative definiteness of $Q(\mu)$, $\mu := 2\sigma_k - \sigma_{k-1}$ is tested (which can be done by computing the Cholesky decomposition of $-Q(\mu)$). For not too small gaps between J_+ and J_- this test often revealed that $Q(\lambda)$ is hyperbolic well before convergence of the safeguarded iteration.
- Although for multiple eigenvalues the quadratic convergence of the safeguarded iteration is not proved the double step strategy worked also fine for double eigenvalues λ_1^+ and λ_1^- (cf. Example 3.3).
- The algorithm fails if the both sequences $\{\sigma_k\}$ and $\{\omega_k\}$ converge and if their limits are very close to each other or even coincide. In the latter case $Q(\lambda)$ is called weakly hyperbolic.

Definition 3.1. The pencil $Q(\lambda)$ is weakly hyperbolic if A, B , and C are Hermitian, $A > 0$, and

$$\gamma := \min_{\|x\|=1} [(x^H B x)^2 - 4(x^H A x)(x^H C x)] \geq 0. \quad (3.5)$$

A weakly hyperbolic eigenvalue problem has $2n$ real eigenvalues, and if $\gamma = 0$ (i.e. $Q(\lambda)$ is not hyperbolic) then it holds that

$$\lambda_n^- \leq \lambda_{n-1}^- \leq \dots \leq \lambda_1^- = \lambda_1^+ \leq \lambda_2^+ \leq \dots \leq \lambda_n^+. \quad (3.6)$$

Obviously, p_+ as defined in (3.3) is a Rayleigh functional of $Q(\lambda)$ with respect to the interval $\tilde{J}_+ := (\lambda_1^+, \infty)$ satisfying (A_1) and (A_2) , and all eigenvalues in \tilde{J}_+ are minmax and maxmin values of p_+ .

If $\sigma_{k-1} \in \tilde{J}_+$, and x_k is an eigenvector corresponding to the maximal eigenvalue of $Q(\sigma_{k-1})$, then (cf. (2.10)) $x_k^H Q(\sigma_{k-1}) x_k \geq 0$, and therefore the maximal solution σ_k of the quadratic equation $x_k^H Q(\lambda) x_k = 0$ satisfies $\sigma_k = p_+(x_k)$ or $\sigma_k = \lambda_1^+$. Hence, the safeguarded iteration stops after a finite number of steps with $\sigma_k = \lambda_1^+$ or $\{\sigma_k\} \subset \tilde{J}_+$ is a monotonically decreasing sequence converging to some $\hat{\sigma} \in \tilde{J}_+$. In the latter case we obtain in the same way as in the proof of Theorem 2.2 that $\hat{\sigma} = \lambda_1^+$. Likewise, the sequence $\{\omega_k\}$ constructed in the same way for the interval $(-\infty, \lambda_1^-)$ converges to λ_1^- and is monotonically increasing.

We now assume that $Q(\lambda)$ is hyperbolic. Once a parameter μ is found such that $Q(\mu)$ is negative definite the following transformation yields a definite linearization of $Q(\lambda)$. Shifting $Q(\lambda)$ by μ yields a quadratic matrix polynomial

$$\tilde{Q}(\lambda) := Q(\lambda + \mu) = \lambda^2 A + \lambda(B + 2\mu A) + (C + \mu^2 A + \mu B) =: \lambda^2 \tilde{A} + \lambda \tilde{B} + \tilde{C},$$

where $\tilde{C} = \tilde{Q}(0) = Q(\mu)$ is negative definite, and the well known linearizations [8,20]

$$L_1(\lambda) := \lambda \begin{pmatrix} \tilde{A} & 0 \\ 0 & -\tilde{C} \end{pmatrix} + \begin{pmatrix} \tilde{B} & \tilde{C} \\ \tilde{C} & 0 \end{pmatrix} \quad \text{and} \quad L_2(\lambda) := \lambda \begin{pmatrix} 0 & \tilde{A} \\ \tilde{A} & \tilde{B} \end{pmatrix} + \begin{pmatrix} -\tilde{A} & 0 \\ 0 & \tilde{C} \end{pmatrix} \quad (3.7)$$

of $\tilde{Q}(\lambda)$ are obviously definite. Employing the Cholesky factorization of $\text{diag}\{\tilde{A}, -\tilde{C}\}$ it can be transformed to a standard eigenvalue problem and solved by the QR algorithm preserving the reality of its eigenvalues.

The k th step of the upper sweep of Algorithm 2 requires $n^3/3$ operations for computing one Cholesky factorization, $4n^2$ operations for evaluating $Q(2\sigma_k - \sigma_{k-1})$, three matrix–vector products ($6n^2$ operations), three scalar products ($6n$ operations), and the determination of the largest eigenvalue and corresponding eigenvector of a matrix $Q(\sigma_{k-1})$, and the lower sweep has a similar complexity.

The most expensive part seems to be the solution of the eigenvalue problem $Q(\sigma_k)x = \mu x$. Notice however, that the matrices $Q(\sigma_k)$ converge as the sequence $\{\sigma_k\}$ converges. Hence, one should reuse as much information as possible from previous steps when solving the eigenvalue problem $Q(\sigma_{k-1})x_k = \mu x_k$. Rayleigh quotient iteration or (implicitly restarted) Krylov subspace methods are able to use the eigenvector x_{k-1} of the last step as initial vector. The nonlinear Arnoldi method [25,33] in Algorithm 3 can use the entire search space of the previous step as initial information. A similar technique was used in [18,19] to accelerate methods for regularized total least squares problems that are based on eigensolvers.

Algorithm 3. Nonlinear Arnoldi method

This algorithm determines an eigenvector corresponding to the maximal eigenvalue μ of $Q(\sigma_k)$ for a given σ_k where $Q(\lambda) = \lambda^2 A + \lambda B + C$, and A, B, C are symmetric

Require: A, B, C, σ_k , preconditioner $PC \approx Q(\sigma_k)^{-1}$, initial basis V with $V^T V = I$

Require: projected matrices $A_V := V^H A V, B_V := V^H B V, C_V := V^H C V$

- 1: find largest eigenvalue μ of $(\sigma_k^2 A_V + \sigma_k B_V + C_V)z = \mu z$ and corresponding eigenvector z
- 2: set $u = Vz, r = (Q(\sigma_k) - \mu I)u$
- 3: **while** $\|r\|/\|u\| > \epsilon$ **do**


```

4:  $v = PCr$ 
5:  $v = v - VV^T v$ 
6: re-orthogonalize if necessary
7:  $\tilde{v} = v / \|v\|$ ,  $V = [V, \tilde{v}]$ 
8: restart if  $\dim(\text{span} V) > \text{maxdim}$ 
9: update projected matrices  $A_V, B_V, C_V$ 
10: find largest eigenvalue  $\mu$  of  $(\sigma_k^2 A_V + \sigma_k B_V + C_V)z = \mu z$  and corresponding eigenvector  $z$ 
11: set  $u = Vz$ ,  $r = (Q(\sigma_k) - \mu I)u$ 
12: end while

```

Since the search spaces are reused their dimensions can become quite large. We restarted the nonlinear Arnoldi method with the one dimensional space spanned by the current eigenvector approximation if the dimension exceeded a predetermined maximal dimension.

In our numerical experiments it turned out that it was not necessary to update the preconditioner PC . Hence, one LU factorization with $2n^3/3$ operations is required.

Moreover, to initialize the nonlinear Arnoldi method the matrix $Q(\sigma_k)$ has to be provided ($4n^2$ operations), the vectors u and r have to be computed requiring $2nm$ and $2n^2$ operations, if m denotes the dimension of the current search space $\text{span}(V)$, and an m dimensional eigenvalue problem has to be solved which requires $16m^3/3 + O(m^2)$ operations with the QR algorithm (cf. [3]).

An inner iteration step of the nonlinear Arnoldi method causes the following cost. Multiplying the residual r by the preconditioner PC requires $2n^2$ operations, the orthogonalization of the expansion vector v against V needs $4nm + 2n$ operations, to update the projected matrices A_V, B_V , and C_V needs $3(2n^2 + 2nm)$ operations, the solution of the m dimensional eigenvalue problem by the QR algorithm costs $16m^3/3 + O(m^2)$ operations, and the computation of the Ritz vector u and the residual r requires $2nm$ and $2n^2$ operations, respectively.

These operation counts refer to full matrices A, B , and C . For banded or general sparse matrices the cost for computing matrix-vector products, the preconditioner and the Cholesky decomposition will be much smaller.

Example 3.1 (cf. [7,9]). Consider the quadratic eigenvalue problem (3.1) of dimension $n = 100$ with $A = I$,

$$B = \beta \begin{pmatrix} 20 & -10 & & & \\ -10 & 30 & -10 & & \\ & \ddots & \ddots & \ddots & \\ & & -10 & 30 & -10 \\ & & & -10 & 20 \end{pmatrix}, \quad C = \begin{pmatrix} 15 & -5 & & & \\ -5 & 15 & -5 & & \\ & \ddots & \ddots & \ddots & \\ & & -5 & 15 & -5 \\ & & & -5 & 15 \end{pmatrix},$$

where β is a real parameter.

For $\beta \geq \beta_u := 0.5196152423$, $Q(\lambda)$ is hyperbolic, and for $\beta \leq \beta_l := 0.5196152422$ it is not hyperbolic. We tested the type of $Q(\lambda)$ for the parameters β_l and β_u . Because the behavior of our method depends on the choice of the initial vector x_0 we solved either type with 20 different initial vectors the components of which are normally distributed pseudo random numbers with mean value 0 and variance 1.

In any case Algorithm 2 detected the correct type of the problem requiring an average CPU time of 0.06 seconds on a Pentium D computer with 3.2 GHz and 2 GB RAM. The maximal dimension of the search space in the nonlinear Arnoldi method was 40, and the minimal dimension was 31, while the average of the dimensions of the required search spaces was 35.5.

Fig. 3.1 contains typical convergence histories of the method for the hyperbolic case (on the left) and the non-hyperbolic case (on the right). The circles mark the residual norms $\|(Q(\sigma_k) - \mu I)x\|$ of the outer iteration (safeguarded iteration) while the straight lines indicate the residual norms within the nonlinear Arnoldi method.

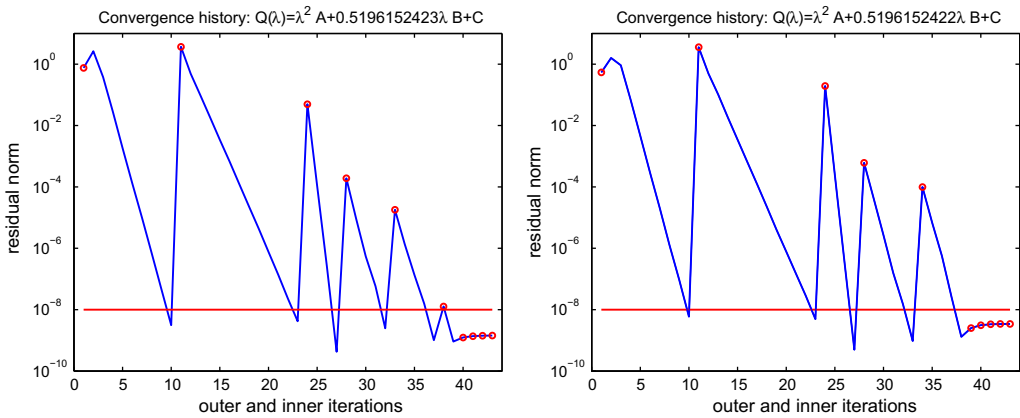


Fig. 3.1. Convergence history for Example 3.1.

It demonstrates that it pays off to reuse the search spaces of previous iteration steps: the first safeguarded iteration step requires a search space of dimension 10, the basis of which is expanded in the following steps by 12, 3, 4, 4, and 1 vectors. After the sixth outer iteration step the search space of dimension 34 is not further expanded, but in the the following four steps of the safeguarded iteration it can be kept fixed.

Example 3.2. We use the following method for constructing quadratic matrix polynomials with prescribed eigenvalues and eigenvectors (cf. [21]): For $(\lambda_j, v_j), j = 1, \dots, 2n$ let

$$\begin{aligned} A_1 &:= \text{diag}\{\lambda_1, \dots, \lambda_n\}, \quad A_2 := \text{diag}\{\lambda_{n+1}, \dots, \lambda_{2n}\}, \\ V_1 &:= [v_1, \dots, v_n], \quad V_2 := [v_{n+1}, \dots, v_{2n}] \in \mathbb{R}^{n \times n}. \end{aligned}$$

Assume that V_1 and V_2 are nonsingular, $V_1 V_1^T = V_2 V_2^T$ and $\Gamma := V_1 A_1 V_1^T - V_2 A_2 V_2^T$ is nonsingular. Then the quadratic polynomial $Q(\lambda)$ with

$$A = \Gamma^{-1}, \quad B = -A(V_1 A_1^3 V_1^T - V_2 A_2^3 V_2^T)A, \quad C = -A(V_1 A_1^3 V_1^T - V_2 A_2^3 V_2^T)A + B\Gamma B$$

has eigenpairs $(\lambda_j, v_j), j = 1, \dots, 2n$.

We constructed a test set of 80 quadratic matrix functions $Q(\lambda) \in \mathbb{R}^{500 \times 500}$ of this type where λ_j , for $j = 1, \dots, 500$ are normally distributed with mean value -3 and standard variation 1, and for $j = 501, \dots, 1000$ λ_j are uniformly distributed in $[-106, -6]$. If $\lambda_{\max} := \max_j \lambda_j > 0$ the eigenvalues λ_j were shifted to the left by $1.1 \lambda_{\max}$ (then all eigenvalues λ_j are negative, and hyperbolic examples are even overdamped [8]; this is not needed in Algorithm 2 but only to compare it to cyclic reduction in [8]). With random orthogonal matrices U_1, U_2 we chose $V_1 = U_1$ and $V_2 = V_1 U_2$ so that $V_1 V_1^T = V_2 V_2^T$. For 51 of these examples $\max_{j=501, \dots, 1000} \lambda_j < \min_{j=1, \dots, 500} \lambda_j$ and the corresponding $Q(\lambda)$ are hyperbolic (actually they are even overdamped, cf. [7]). For the remaining 29 problems the matrix A turned out to be positive definite, but $Q(\lambda)$ was not hyperbolic.

Algorithm 2 detected the type of $Q(\lambda)$ in all examples correctly. The average CPU time was 0.65 s (minimal 0.47, and maximal 1.05 s). The safeguarded iteration required at least two steps, at most three steps, and the average number of steps was 2.06. The nonlinear Arnoldi method constructed search spaces of minimal dimension 31, maximal dimension 67, and the average dimension was 44.8. Since we allowed for a maximal dimension 100 of search spaces no restarts were necessary.

The cyclic reduction algorithm of Guo et al. [7] detected the type of the pencils also in all cases correctly. It required at most 23 and at least no iteration with an average of 8.95, and the average CPU time was 2.55 s (minimal 0.27 and maximal 6.19 s). In 61 (resp. 28 non-hyperbolic) examples the

Table 3.1

Relative errors of the safeguarded iteration for a double eigenvalue.

Iteration	0	1	2	3	4	5
Error	2.4e−1	1.7e−2	2.6e−4	1.5e−7	4.6e−11	1.0e−15

safeguarded iteration was faster, whereas in 19 (resp. 1 non-hyperbolic) examples the cyclic reduction was the winner.

Example 3.3. To evaluate the behavior of our method in case of multiple extreme eigenvalues we constructed test problems in a similar way as in Example 3.2. We modified uniformly distributed numbers λ_j with $-100 \leq \lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_{1000} \leq 0$ by setting $\lambda_{500} := \lambda_{499}$ and $\lambda_{501} := \lambda_{502} := \lambda_{499} + \delta$, and constructed the matrices A, B and C as described in Example 3.2. Then the resulting quadratic eigenvalue problem $Q(\lambda)$ is hyperbolic, the extreme eigenvalues λ_1^+ and λ_1^- are both double eigenvalues, and the gap $\lambda_1^+ - \lambda_1^- = \delta$.

For $\delta = 10^{-j}$, $j = 1, \dots, 11$ (i.e. for relative gaps between 2×10^{-3} and 2×10^{-13}) our method detected the hyperbolicity of $Q(\lambda)$ correctly, as did the cyclic reduction. The safeguarded iteration required at least three iterations and at most five iterations, and for all $\delta \geq 10^{-10}$ the gap was found in the upper sweep of Algorithm 2, only for $\delta = 10^{-11}$ the lower sweep approximating λ_1^- was needed.

The average CPU time was 2.87 s (minimal 1.49 and maximal 5.59 s) for Algorithm 2 and 6.29 s (minimal 1.60 and maximal 11.27 s) for cyclic reduction. In all cases Algorithm 2 was the winner.

The safeguarded iteration is not known to be quadratically convergent for multiple eigenvalues, but our numerical examples indicated that this might be the case. For example, for $\delta = 10^{-6}$ we obtained the relative errors of σ_k in Table 3.1.

4. Definite quadratic matrix polynomials

In a recent paper Higham et al. [11] generalized the concept of hyperbolic quadratic polynomials waiving the positive definiteness of the leading matrix A .

Definition 4.1. The quadratic matrix polynomial

$$Q(\lambda) := \lambda^2 A + \lambda B + C \quad (4.1)$$

is definite if $A = A^H$, $B = B^H$, $C = C^H$ are Hermitian, there exists $\mu \in \mathbb{R} \cup \{\infty\}$ such that $Q(\mu)$ is positive definite, and for every fixed $x \neq 0$ the real equation

$$f(\lambda; x) := \lambda^2 x^H A x + \lambda x^H B x + x^H C x = 0 \quad (4.2)$$

has two distinct roots in $\mathbb{R} \cup \{\infty\}$.

The following Theorem was proved in [11].

Theorem 4.2. The Hermitian matrix polynomial $Q(\lambda)$ is definite if and only if any two (and hence all) of the following properties hold:

- $d(x) := (x^H B x)^2 - 4(x^H A x)(x^H C x) > 0$ for every $x \in \mathbb{C}^n \setminus \{0\}$,
- $Q(\eta) > 0$ for some $\eta \in \mathbb{R} \cup \{\infty\}$,
- $Q(\xi) < 0$ for some $\xi \in \mathbb{R} \cup \{\infty\}$.

Hence, to detect that a pencil is definite we have to find $\xi, \eta \in \mathbb{R} \cup \{\infty\}$ such that $Q(\xi) < 0 < Q(\eta)$.

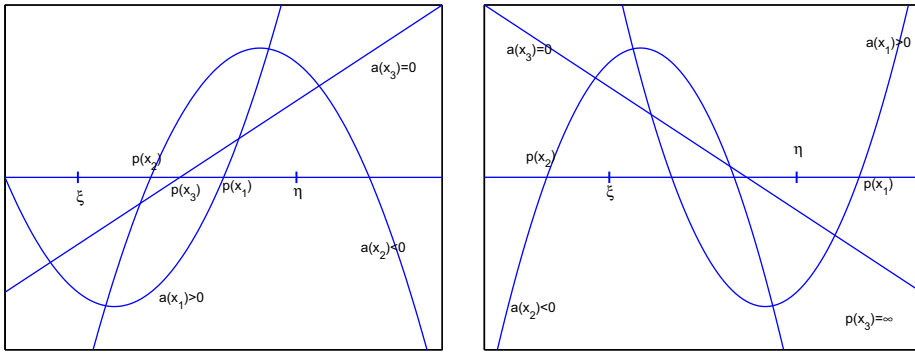


Fig. 4.1. Definition of p for definite quadratic matrix polynomials; case $Q(\xi) < 0 < Q(\eta)$ on the left and case $Q(\xi) > 0 > Q(\eta)$ on the right. $x_j, j = 1, 2, 3$ are typical points with $a(x_1) > 0$, $a(x_2) < 0$, and $a(x_3) = 0$.

Assume that $Q(\lambda)$ is definite, and consider first the case that $\xi < \eta \leq \infty$ and $Q(\xi) < 0 < Q(\eta)$. Then for every $x \in \mathbb{C}^n$, $x \neq 0$ the quadratic equation (4.2) has a unique solution $p(x) \in J := (\xi, \eta)$, and it follows from $x^H Q(\xi)x < 0$ that the condition

$$(\lambda - p(x))f(\lambda; x) > 0 \quad \text{for every } \lambda \in J, \lambda \neq p(x)$$

is satisfied.

Obviously, the Rayleigh functional is explicitly given by (cf. the left picture in Fig. 4.1)

$$p(x) = \begin{cases} -\frac{b(x)}{2a(x)} + \sqrt{\left(\frac{b(x)}{2a(x)}\right)^2 - \frac{c(x)}{a(x)}} & \text{if } a(x) > 0, \\ -\frac{c(x)}{b(x)} & \text{if } a(x) = 0, \\ -\frac{b(x)}{2a(x)} - \sqrt{\left(\frac{b(x)}{2a(x)}\right)^2 - \frac{c(x)}{a(x)}} & \text{if } a(x) < 0, \end{cases} \quad (4.3)$$

where $a(x) := x^H A x$, $b(x) := x^H B x$, and $c(x) := x^H C x$.

The quadratic eigenvalue problem $Q(\lambda)x = 0$ has exactly n eigenvalues $\lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_n$ in J which satisfy a minmax characterization with respect to p , and the safeguarded iterations aiming at λ_1 and λ_n converge globally and monotonically and are decreasing and increasing, respectively.

Conversely, consider the case that $-\infty < \xi < \eta \leq \infty$ and $Q(\xi) > 0 > Q(\eta)$ (cf. Fig. 4.1 on the right). Then the considerations in the first case hold for the matrix polynomial $-Q(\lambda)$, and therefore $Q(\lambda)x = 0$ has exactly n eigenvalues in (ξ, η) , and the remaining n eigenvalues are contained in $(-\infty, \xi) \cup (\eta, \infty]$.

For $a(x) \neq 0$

$$p(x) \in ((-\infty, \xi) \cup (\eta, \infty)) \quad (4.4)$$

and for $a(x) = 0$ the equation $x^H Q(\lambda)x = 0$ has a unique real root which is lying in (ξ, η) . We therefore modify the definition of p in the following way

$$p(x) = \begin{cases} -c(x)/b(x) & \text{if } a(x) = 0, b(x) > 0, \\ \infty & \text{if } a(x) = 0, b(x) < 0, \end{cases} \quad (4.5)$$

such that

$$p(\mathbb{C}^n \setminus \{0\}) \subset ((-\infty, \xi) \cup (\eta, \infty]).$$

Three cases are possible:

- (i) There are no eigenvalues in (η, ∞) . Then problem (4.1) has n eigenvalues in $[-\infty, \xi)$. The largest of these eigenvalues is an n th eigenvalue λ_n , since $Q(\xi)$ is positive definite, and it follows from

the continuous dependence of the eigenvalues of $Q(\lambda)$ on λ that 0 is the smallest eigenvalue of $Q(\lambda_n)$. The eigenvalues in $(-\infty, \xi)$ can be characterized as maxmin values of p , and the safeguarded iteration aiming at λ_n converges globally to λ_n and is monotonically increasing. If the minimal eigenvalue λ_1 is finite, then the safeguarded iteration aiming at λ_1 converges monotonically to λ_1 and is decreasing, otherwise the sequence $\{\sigma_k\}$ is monotonically decreasing and unbounded.

- (ii) There are no eigenvalues in $(-\infty, \xi)$. Then similarly (4.1) has n eigenvalues $\eta < \lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_n \leq \infty$, the finite ones of which can be characterized as minmax values of p . The safeguarded iteration aiming at the smallest eigenvalue converges globally and monotonically to λ_1 and is decreasing, and aiming at the largest eigenvalue it is monotonically increasing, and it converges to λ_n if $\lambda_n < \infty$, and otherwise the sequence $\{\sigma_k\}$ is unbounded.
- (iii) There exist finite eigenvalues left and right of the interval $[\xi, \eta]$. Then the restriction of p to the set $\{x \in \mathbb{C}^n : p(x) < \xi\}$ satisfies the conditions of the maxmin characterization, and in particular $\lambda_n := \max_{p(x) < \xi, x \neq 0} p(x)$ is the largest eigenvalue of (4.1) less than ξ , and the restriction of p to the set $\{x \in \mathbb{C}^n : p(x) > \eta\}$ satisfies the conditions of the minmax characterization, and in particular $\lambda_1 := \min_{p(x) > \eta, x \neq 0} p(x)$ is the smallest eigenvalue of (4.1) greater than η . The safeguarded iteration aiming at λ_1 is globally convergent and monotonically decreasing in a generalized sense. For $\sigma_0 \in (\eta, \infty]$ it has the same behavior as in case (i). For $\sigma_0 < \xi$ the following Lemma 4.3 demonstrates that after a finite number of steps the sequence $\{\sigma_k\}$ jumps into the interval $(\eta, \infty]$, and then it converges monotonically to λ_1 and is decreasing.

Lemma 4.3. *Let $Q(\lambda)$ be definite, let $Q(\xi) > 0 > Q(\eta)$ for $\xi < \eta$, and assume that there exist finite eigenvalues on either side of the interval $[\xi, \eta]$. Let $\sigma_0 < \xi$, and $\{\sigma_k\}$ be the sequence constructed by safeguarded iteration for computing a first eigenvalue λ_1 . Then there exists $j \in \mathbb{N}$ such that $\xi > \sigma_0 \geq \sigma_1 \geq \dots \geq \sigma_{j-1} > -\infty$, $\sigma_j \in (\eta, \infty]$, and $\{\sigma_k\}$, $k \geq j$ converges monotonically to $\lambda_1 = \min_{x \neq 0, p(x) > \eta} p(x)$ and is decreasing.*

Proof. For $\sigma_{j-1} \in (-\infty, \xi)$ one gets in the same way as in (2.10) $\mu_n(\sigma_{j-1}) \geq 0$, and $\mu_n(\sigma_{j-1}) = 0$ implies that σ_{j-1} is a first eigenvalue, and there are no eigenvalues in (η, ∞) . Hence, $\mu_n(\sigma_{j-1}) > 0$, and it follows from (A₂) that either $\sigma_j \in (\eta, \infty]$ (and we are done) or $-\infty < \sigma_j < \sigma_{j-1}$.

If $\{\sigma_k\} \subset (-\infty, \xi)$ has a finite limit $\hat{\sigma}$ then it follows in the same way as in proof of Theorem 2.2 that $\hat{\sigma}$ is a first eigenvalue contradicting that there exists an eigenvalue in (η, ∞) .

Finally assume that $\lim_{k \rightarrow \infty} \sigma_k = -\infty$. Let $\{x_{k_j}\}$ be a convergent subsequence of $\{x_k\}$ with $\hat{x} = \lim_{j \rightarrow \infty} x_{k_j}$. Then it holds that

$$0 = \lim_{j \rightarrow \infty} \frac{1}{2} x_{k_j}^H Q(\sigma_{k_j}) x_{k_j} = \lim_{j \rightarrow \infty} \left(x_{k_j}^H A x_{k_j} + \frac{1}{\sigma_{k_j}} x_{k_j}^H B x_{k_j} + \frac{1}{\sigma_{k_j}^2} x_{k_j}^H C x_{k_j} \right) = \hat{x}^H A \hat{x}.$$

Moreover,

$$\lim_{j \rightarrow \infty} \frac{1}{\sigma_{k_j-1}^2} \mu_n(\sigma_{k_j-1}) = \lim_{j \rightarrow \infty} \frac{1}{\sigma_{k_j-1}^2} x_{k_j}^H Q(\sigma_{k_j-1}) x_{k_j} = \hat{x}^H A \hat{x} = 0,$$

which implies that

$$A \hat{x} = \lim_{j \rightarrow \infty} \frac{1}{\sigma_{k_j-1}^2} Q(\sigma_{k_j-1}) x_{k_j} = \lim_{j \rightarrow \infty} \frac{1}{\sigma_{k_j-1}^2} \mu_n(\sigma_{k_j-1}) x_{k_j} = 0.$$

Hence, \hat{x} is an eigenvector of $Q(\infty)$, and

$$\lim_{j \rightarrow \infty} \frac{1}{\sigma_{k_j-1}^2} \mu_n(\sigma_{k_j-1}) = \lim_{j \rightarrow \infty} \max_{\|x\|=1} (x^H A x + \frac{1}{\sigma_{k_j-1}} x^H B x + \frac{1}{\sigma_{k_j-1}^2} x^H C x) = \mu_n(A) = 0$$

demonstrating that $\lambda_1(Q) = \infty$ such that there is no eigenvalue in (η, ∞) . \square

In cases (i) and (ii) the safeguarded iteration aiming at λ_1 and λ_n converges globally and monotonically to $\lambda_1 := \min_{x \neq 0} p(x)$ and $\lambda_n := \max_{x \neq 0} p(x)$ and is decreasing and increasing, respectively.

The same holds true in case (iii) in a generalized sense: Aiming at λ_1 the sequence σ_k may start in $(-\infty, \xi)$, decrease until after a finite number of steps it jumps into (η, ∞) , and then converges monotonically to λ_1 and is decreasing. Similarly, the safeguarded iteration for determining λ_n may start in (η, ∞) , jump into $(-\infty, \xi)$ after some steps, and converge monotonically increasing to λ_n .

In any case the safeguarded iteration for computing the eigenvalue λ_1 converges monotonically and is decreasing, and the one for computing the eigenvalue λ_n converges monotonically and is increasing, possibly in the generalized sense of the last paragraph.

Hence, if $Q(\lambda)$ is definite we can determine by Algorithm 2 a parameter ξ such that $Q(\xi)$ is negative definite. We only have to replace p_+ by p in (4.3) with modification (4.5), and we have to allow for one violation of the monotonicity requirement to incorporate the possible jump of the iterates from one unbounded interval to the other. A second similar sweep aiming at λ_n discovers a parameter η such that $Q(\eta) > 0$.

If $|(\sigma_k - \sigma_{k-1})/\sigma_k|$ in line 11 becomes small then the lower sweep of Algorithm 2 (lines 20–35) is run where p_- is replaced by the functional

$$q(x) = \begin{cases} -\frac{b(x)}{2a(x)} - \sqrt{\left(\frac{b(x)}{2a(x)}\right)^2 - \frac{c(x)}{a(x)}} & \text{if } a(x) > 0, \\ -c(x)/b(x) & \text{if } a(x) = 0, b(x) < 0, \\ \infty & \text{if } a(x) = 0, b(x) > 0, \\ -\frac{b(x)}{2a(x)} + \sqrt{\left(\frac{b(x)}{2a(x)}\right)^2 - \frac{c(x)}{a(x)}} & \text{if } a(x) < 0. \end{cases} \quad (4.6)$$

Once parameters ξ and η are found such that $Q(\xi) < 0 < Q(\eta)$ a definite linearization can be determined similarly to the hyperbolic case (cf. [11]). One first transforms the homogeneous form of $Q(\lambda)$

$$Q(\alpha, \beta) = \alpha^2 A + \alpha\beta B + \beta^2 C, \quad \alpha^2 + \beta^2 = 1, \quad \lambda = \frac{\alpha}{\beta} \quad (4.7)$$

by a plane rotation

$$\begin{pmatrix} \alpha \\ \beta \end{pmatrix} = \begin{pmatrix} c & -s \\ s & c \end{pmatrix} \begin{pmatrix} \tilde{\alpha} \\ \tilde{\beta} \end{pmatrix}, \quad c^2 + s^2 = 1, \quad (4.8)$$

such that η is mapped to ∞ . Then the rotated $\tilde{Q}(\lambda)$ is hyperbolic and can be linearized as in Section 3.

Example 4.1. We modified the test set of Example 3.2 in the following way. We rotated the homogeneous form of a quadratic matrix polynomial by a random angle and obtained a quadratic matrix polynomial

$$\tilde{Q}(\lambda) = \lambda^2(c^2A + csB + s^2C) + \lambda(-2csA + (c^2 - s^2)B + 2csC) + (s^2A - csB + c^2C),$$

with $\lambda = \tilde{\alpha}/\tilde{\beta}$ which has the same spectral properties as $Q(\lambda)$. Hence, $\tilde{Q}(\lambda)$ is definite if and only if $Q(\lambda)$ is hyperbolic.

Then the modified test set of Example 3.2 consists of 51 definite matrix polynomials and 29 quadratic pencils which are not definite.

Our Algorithm detected the type of the matrix polynomial in all cases correctly. The average CPU time was 1.14 s. The safeguarded iteration required at least two steps, at most five steps, and the average number of steps was 2.51. The nonlinear Arnoldi method constructed search spaces of minimal dimension 32. The maximum number of expansions of the search space was 516, and the average number of inner iterations was 82.4. We restarted if the dimension exceeded 100, which was necessary in five examples.

5. Hyperbolic matrix polynomials

The Hermitian matrix polynomial

$$P(\lambda) = \sum_{j=0}^{\ell} \lambda^j A_j, \quad A_j = A_j^H \in \mathbb{C}^{n \times n}, \quad A_{\ell} \neq 0 \quad (5.1)$$

is hyperbolic if A_{ℓ} is positive definite, and for every $x \in \mathbb{C}^n$, $x \neq 0$ the scalar polynomial $q(\lambda; x) := x^H P(\lambda)x$ has ℓ distinct real roots.

The following characterization of hyperbolicity was shown by Markus [24].

Theorem 5.1. *Let $P(\lambda)$ be a Hermitian matrix polynomial of degree $\ell > 1$ with positive definite A_{ℓ} . Then $P(\lambda)$ is hyperbolic if and only if there exist $\gamma_j \in \mathbb{R}$ such that*

$$\gamma_1 > \gamma_2 > \cdots > \gamma_{\ell-1} \quad \text{and} \quad (-1)^j P(\gamma_j) > 0, \quad j = 1, \dots, \ell - 1. \quad (5.2)$$

From $A_{\ell} > 0$ it follows that there exists $\gamma_0 > \gamma_1$ such that $P(\gamma_0) > 0$, and $P(\gamma_1) < 0$ yields that

$$p_1(x) := \max\{\mu \in \mathbb{R} : x^H P(\mu)x = 0\}, \quad x \neq 0$$

defines a Rayleigh functional of $P(\lambda)x = 0$ corresponding to the interval (γ_1, ∞) . Obviously, p_1 is defined on $\mathbb{C}^n \setminus \{0\}$, and the sign condition (A_2) is satisfied. Hence, the nonlinear eigenvalue problem $P(\lambda)x = 0$ has n eigenvalues $\lambda_j^{(1)}$ with

$$\gamma_1 < \lambda_1^{(1)} \leq \lambda_2^{(1)} \leq \cdots \leq \lambda_n^{(1)} < \infty$$

and

$$\lambda_j^{(1)} = \min_{\dim V=j} \max_{x \in V, x \neq 0} p_1(x).$$

From $P(\gamma_1) < 0 < P(\gamma_2)$ it follows that

$$p_2(x) := \max\{\mu < \gamma_1 : x^H P(\mu)x = 0\}, \quad x \neq 0$$

defines a Rayleigh functional of $-P(\lambda)x = 0$ corresponding to the interval (γ_2, γ_1) which is defined on $\mathbb{C}^n \setminus \{0\}$, and satisfies the sign condition (A_2) .

Hence, $P(\lambda)x = 0$ has n eigenvalues

$$\gamma_2 < \lambda_n^{(2)} \leq \lambda_{n-1}^{(2)} \leq \cdots \leq \lambda_1^{(2)} < \gamma_1$$

and

$$\lambda_j^{(2)} = \max_{\dim V=j} \min_{x \in V, x \neq 0} p_2(x).$$

Likewise, for each of the intervals (γ_k, γ_{k-1}) , $k = 1, \dots, \ell$ with $\gamma_{\ell} = -\infty$

$$p_k(x) := \max\{\mu \leq \gamma_{k-1} : x^H P(\mu)x = 0\}, \quad x \neq 0$$

defines a Rayleigh functional of $\pm P(\lambda)x = 0$.

In (γ_k, γ_{k-1}) there are exactly n eigenvalues. For odd k it holds that

$$\gamma_k < \lambda_1^{(k)} \leq \lambda_2^{(k)} \leq \cdots \leq \lambda_n^{(k)} < \gamma_{k-1},$$

$$\lambda_j^{(k)} = \min_{\dim V=j} \max_{x \in V, x \neq 0} p_k(x)$$

and for even k

$$\gamma_k < \lambda_n^{(k)} \leq \lambda_{n-1}^{(k)} \leq \cdots \leq \lambda_1^{(k)} < \gamma_{k-1},$$

$$\lambda_j^{(k)} = \max_{\dim V=j} \min_{x \in V, x \neq 0} p_k(x).$$

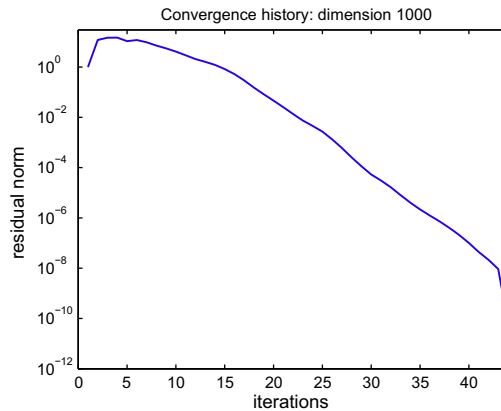


Fig. 5.1. Convergence history for hyperbolic cubic matrix polynomial.

These results suggest the following approach for detecting the hyperbolicity of a matrix polynomial $P(\lambda)$.

Assume that A_ℓ is positive definite. For a given initial vector $x_0 \neq 0$ and $\sigma_0 = p_1(x_0)$, we determine $\lambda_1^{(1)} = \inf p_1(x)$ by the safeguarded iteration for p_1 , i.e. $\sigma_i = p_1(x_i)$ where x_i is an eigenvector corresponding to the largest eigenvalue of $P(\sigma_{i-1})$.

Having found $\lambda_1^{(1)}$ and having tested whether $P(\gamma_2)$, $\gamma_2 := \lambda_1^{(1)} - \epsilon$ is negative definite for sufficiently small $\epsilon > 0$, determine $\lambda_n^{(2)}$ by the safeguarded iteration for p_2 , i.e. $\sigma_i = p_2(x_i)$ where x_i is an eigenvector corresponding to the smallest (notice that in this interval $-P(\lambda)$ satisfies the conditions of Theorem 2.2) eigenvalue of $P(\sigma_{i-1})$.

Treat the following intervals analogously determining the smallest eigenvalue by safeguarded iteration and checking the positive definiteness of $(-1)^j P(\gamma_j)$, $\gamma_j := \lambda_{\min} - \epsilon$ for sufficiently small $\epsilon > 0$.

The method can be terminated if one of the polynomials $q(\lambda; x_i) := x_i^H P(\lambda) x_i$ has less than ℓ distinct real roots or if the sequence $\{\sigma_i\}$ is not monotonically decreasing, since then $P(\lambda)$ is not hyperbolic.

As for the quadratic case special care has to be taken to recognize weak hyperbolicity, and an additional safeguarded iteration aiming at the maximal eigenvalue in (γ_j, γ_{j-1}) may be necessary if $P(\lambda_{\min} - \epsilon)$ is ill-conditioned for some j (cf. the remarks about the lower sweep of Algorithm 2 in Section 3). After parameters $\gamma_j, j = 1, \dots, \ell - 1$ satisfying (5.2) have been found and $\gamma_0 > \gamma_1$ has been chosen such that $P(\gamma_0) > 0$, a definite linearization can be constructed as suggested by Higham et al. [11].

Example 5.2. For a hyperbolic cubic matrix polynomial

$$P(\lambda) = \lambda^3 A + \lambda^2 B + \lambda C + D,$$

where the three intervals $[\lambda_1^{(3)}, \lambda_n^{(3)}]$, $[\lambda_n^{(2)}, \lambda_1^{(2)}]$, and $[\lambda_1^{(1)}, \lambda_n^{(1)}]$ are well separated, Fig. 5.1 shows the typical convergence behavior of our approach. The method detects a point $\gamma_1 = \lambda_1^{(1)} - \epsilon$ such that $P(\gamma_1)$ is negative definite with a search space of moderate dimension, and with the same search space aiming at $\lambda_n^{(2)}$ one immediately finds γ_2 with $P(\gamma_2) > 0$. Here $A = I$ and B, C , and D are sparse matrices of dimension $n = 1000$ (each with approximately 20,000 non-zero elements) and the CPU time for identifying hyperbolicity is 1.8 s.

We modified the example multiplying the negative definite matrix C by a real parameter β . For $\beta = 0.63116944193$ the matrix polynomial is hyperbolic with a small gap $\lambda_n^{(2)} - \lambda_n^{(3)} = 2.0e-5$ between the second and third group of n eigenvalues. The method determined γ_1 with $P(\gamma_1) < 0$ with one

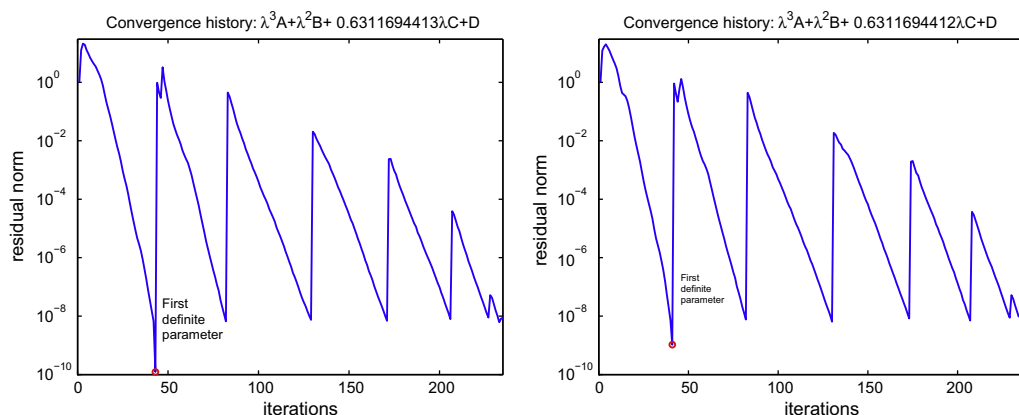


Fig. 5.2. Convergence history for Example 5.1.

safeguarded iteration step and a search space of dimension 42. To find $\gamma_2 \in (\lambda_n^{(3)}, \lambda_n^{(2)})$ with $P(\gamma_2) > 0$ it took 10 steps of the safeguarded iteration and a 225 dimensional search space (cf. Fig. 5.2 on the left) and a total CPU time of 19.5 s.

$P(\lambda)$ with $\beta = 0.63116944192$ is not hyperbolic. The convergence behaviour is shown in the right picture of Fig. 5.2, 19.7 s CPU time were needed.

6. Definite matrix polynomials

Definition 6.1. A Hermitian matrix polynomial $P(\lambda) = \sum_{j=0}^{\ell} \lambda^j A_j$ is called definite if there exists $\mu \in \mathbb{R} \cup \{\infty\}$ such that $P(\mu)$ is positive definite and for every $x \in \mathbb{C}^n$, $x \neq 0$ the scalar polynomial $q(\lambda; x) := x^H P(\lambda) x$ has ℓ distinct roots in $\mathbb{R} \cup \{\infty\}$.

The spectral properties of a definite polynomial can be most easily obtained by rotation of the homogeneous form

$$P(\alpha, \beta) = \sum_{j=0}^{\ell} \alpha^j \beta^{\ell-j} A_j, \quad \lambda := \frac{\alpha}{\beta}, \quad \alpha^2 + \beta^2 = 1 \quad (6.1)$$

of $P(\lambda)$.

For the rotated polynomial

$$\begin{aligned} P(\alpha, \beta) &= \sum_{j=0}^{\ell} \alpha^j \beta^{\ell-j} A_j = \sum_{j=0}^{\ell} (c\tilde{\alpha} - s\tilde{\beta})^j (s\tilde{\alpha} + c\tilde{\beta})^{\ell-j} \tilde{A}_j \\ &=: \sum_{j=0}^{\ell} \tilde{\alpha}^j \tilde{\beta}^{\ell-j} \tilde{A}_j =: \tilde{P}(\tilde{\alpha}, \tilde{\beta}) \end{aligned} \quad (6.2)$$

using the plane rotation (4.8) it holds that the eigenvectors of P and \tilde{P} are the same, that the corresponding eigenvalues are rotated, and that $x^H P(\alpha, \beta) x = x^H \tilde{P}(\tilde{\alpha}, \tilde{\beta}) x$ for every $x \in \mathbb{C}$. Moreover,

$$\tilde{A}_{\ell} = \tilde{P}(1, 0) = P(c, s) \quad \text{and} \quad \tilde{A}_0 = \tilde{P}(0, 1) = P(-s, c).$$

Now rotate μ into ∞ . Then $\tilde{A}_{\ell} = \tilde{P}(1, 0) = P(\mu)$ is positive definite, and $x^H \tilde{P}(\tilde{\lambda}) x = x^H P(\lambda) x = 0$ has ℓ distinct roots in $\mathbb{R} \cup \{\infty\}$ for every $x \in \mathbb{C}^n$, $x \neq 0$. Hence, \tilde{P} is hyperbolic, and there exist $\tilde{\gamma}_j \in \mathbb{R}$, $j = 1, \dots, \ell$ such that $\tilde{\gamma}_{\ell} < \dots < \tilde{\gamma}_1 < \tilde{\gamma}_0 := \infty$ and $(-1)^j \tilde{P}(\tilde{\gamma}_j)$ is positive definite for every $j = 0, \dots, \ell$.

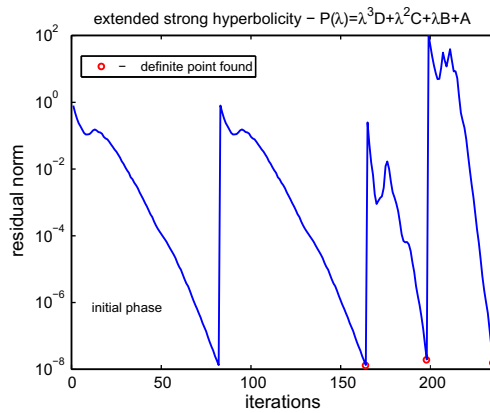


Fig. 6.1. Convergence history for definite cubic matrix polynomial.

Therefore, in every interval $\tilde{I}_j := (\tilde{\gamma}_j, \tilde{\gamma}_{j-1})$, $j = 1, \dots, \ell$ there are exactly n eigenvalues which allow for a variational characterization with an appropriate Rayleigh functional \tilde{p}_j , and it holds that $x^H \tilde{P}'(\tilde{p}_j(x))x$ is of constant sign.

Rotating back we obtain for the original polynomial P that there are $\gamma_\ell < \gamma_{\ell-1} < \dots < \gamma_1$ such that in every interval $I_j := (\gamma_{j+1}, \gamma_j)$, $j = 1, \dots, \ell - 1$ there are exactly n eigenvalues which allow for a variational characterization with an appropriate Rayleigh functional p_j , and it holds that $x^H P'(p_j(x))x$ is of constant sign. Additionally, there are n more eigenvalues in $(-\infty, \gamma_\ell) \cup (\gamma_1, \infty) \cup \{\infty\}$ the finite of which satisfy variational characterizations with Rayleigh functionals p_ℓ and p_0 corresponding to $I_\ell := (-\infty, \gamma_\ell)$ and to $I_0 := (\gamma_1, \infty)$, respectively.

Let $P(\lambda)$ be a definite polynomial. Let $x_0 \neq 0$, and let σ_0 be the maximal root of the polynomial $x_0^H P(\lambda) x_0$. Then either $\sigma_0 \in I_0$ or $\sigma_0 \in I_1$. We assume without loss of generality that $x_0^H P'(\sigma_0) x_0 > 0$ (otherwise we replace $P(\lambda)$ by $-P(\lambda)$).

Let x_1 denote an eigenvector corresponding to the smallest eigenvalue of $P(\sigma_0)$ and σ_1 be the maximal root of $x_1^H P(\lambda) x_1 = 0$.

If $\sigma_0 \in I_1$, then $p_1(x_1) \geq \sigma_0$, and if $\sigma_0 \in I_0$, then $p_0(x_1) > \sigma_0$ or $p_0(x_1)$ is not defined. Hence, $\sigma_1 < \sigma_0$ implies $\sigma_1 \in I_1$ and $\sigma_0 \in I_0$.

If $\sigma_1 \geq \sigma_0$ and $x_1^H P'(\sigma_1) x_1 < 0$ then it follows that $\sigma_0 \in I_1$ and $\sigma_1 \in I_0$.

Assume that $\sigma_1 \geq \sigma_0$ and $x_1^H P'(\sigma_1) x_1 > 0$. Repeating the procedure above iteratively we finally detect two points $\tau \in I_0$ and $\sigma \in I_1$, or the sequence $\{\sigma_k\}$ converges to the maximal eigenvalue $\lambda_1^{(0)}$ in I_0 .

In the latter case the second largest root σ of $x^H P(\lambda) x$ is contained in I_1 .

Once we have constructed bounds τ and σ for γ_1 we can continue as for the hyperbolic polynomial.

Again the method can be terminated if one of the polynomials $q(\lambda; x_i) := x_i^H P(\lambda) x_i$ has a non-real root or if the sequence $\{\sigma_i\}$ is not monotonically decreasing, since then $P(\lambda)$ is not definite.

Example 6.2. We consider the cubic matrix polynomial

$$P(\lambda) = \lambda^3 D + \lambda^2 C + \lambda B + A$$

with the same matrices as in Example 5.2. Since D is indefinite this matrix polynomial is definite but not hyperbolic.

The convergence behavior is shown in Fig. 6.1. After one step of safeguarded iteration (81 nonlinear Arnoldi steps) the method has found an inclusion of γ_1 and detected that $P(\gamma_1)$ is negative definite. Thereafter, for each of the parameters it took only one safeguarded iteration step to find γ_j , $j = 1, 2, 3$ such that $P(\gamma_1) < 0$, $P(\gamma_2) > 0$ and $P(\gamma_3) < 0$, where the search space had to be expanded by 81, 34, and 36 vectors, respectively.

Acknowledgement

The authors would like to thank an anonymous referee for comments, which considerably improved the presentation of the paper.

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